

=> d his

(FILE 'HOME' ENTERED AT 17:39:41 ON 07 MAR 2002)

FILE 'REGISTRY' ENTERED AT 17:39:52 ON 07 MAR 2002
ACT BER732P/A

L1 STR
L2 36 SEA FILE=REGISTRY SSS FUL L1

L3 1 S L2 AND N=3 *1 compound*

FILE 'HCAPLUS' ENTERED AT 17:40:26 ON 07 MAR 2002

L4 1 S L3 *1 cite*

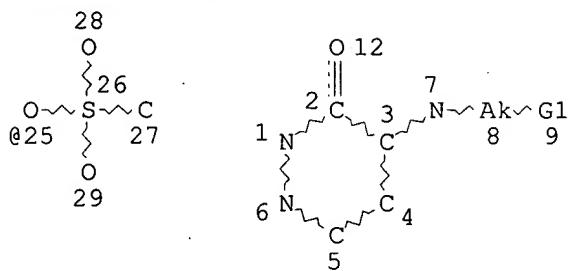
FILE 'CAOLD' ENTERED AT 17:41:54 ON 07 MAR 2002

L5 0 S L3 *no cites*

FILE 'BEILSTEIN' ENTERED AT 17:42:22 ON 07 MAR 2002

L6 0 S L1 FUL *no compounds*

Y> dialogue 14
STR



N~~Ak~~C
21 22 23

this is the related product which I got rid of by limiting n=3 in L3

VAR G1=X/25/21

NODE ATTRIBUTES:

NSPEC IS RC AT 23
 NSPEC IS RC AT 27
 CONNECT IS E2 RC AT 1
 CONNECT IS E2 RC AT 6
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS X5 C AT 8
 ECOUNT IS X5 C AT 22

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

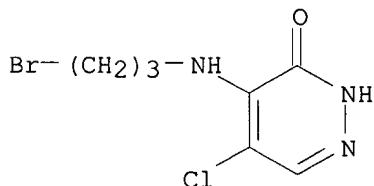
STEREO ATTRIBUTES: NONE

L2 36 SEA FILE=REGISTRY SSS FUL L1
 L3 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND N=3
 L4 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d ibib abs hitstr

PL4 ANSWER 1 OF 1 HCAPLUS • COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:795795 HCAPLUS
 DOCUMENT NUMBER: 132:22970
 TITLE: Preparation of 5-chloro-4-[3-[N-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propylamino]-3(2H)-pyridazinone
 INVENTOR(S): Kotay Nagy, Peter; Simig, Gyula; Barkoczy, Jozsef; Sztruhar, Ilona; Balazs, Laszlo; Doman, Imre; Greff, Zoltan; Ratkai, Zoltan; Seres, Peter; Karancsi, Tamas
 PATENT ASSIGNEE(S): Egis Gyogyszergyar Rt., Hung.
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964402	A1	19991216	WO 1998-HU54	19980605
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9877834	A1	19991230	AU 1998-77834	19980605
EP 1082309	A1	20010314	EP 1998-925869	19980605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2000006183	A	20010130	NO 2000-6183	20001205
PRIORITY APPLN. INFO.:			WO 1998-HU54	A 19980605
OTHER SOURCE(S):		CASREACT 132:22970; MARPAT 132:22970		
AB	Amination of 3,4,5-trichloropyridazine (prepn. given) by H2N(CH2)3OH gave a separable mixt. of 5- and 4-aminated derivs. and the latter was converted to the title compd. in 3 addnl. steps.			
IT	252031-70-2P			
RL	IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)			
	(prepn. of 5-chloro-4-[3-[N-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propylamino]-3(2H)-pyridazinone)			
RN	252031-70-2 HCAPLUS			
CN	3(2H)-Pyridazinone, 4-[(3-bromopropyl)amino]-5-chloro- (9CI) (CA INDEX NAME)			



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

BERNHARDT 09/701,732

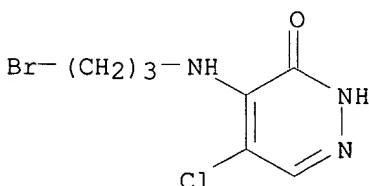
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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PLH ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:795795 HCAPLUS
 DOCUMENT NUMBER: 132:22970
 TITLE: Preparation of 5-chloro-4-[3-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propylamino]-3(2H)-pyridazinone
 INVENTOR(S): Kotay Nagy, Peter; Simig, Gyula; Barkoczy, Jozsef; Sztruhar, Ilona; Balazs, Laszlo; Doman, Imre; Greff, Zoltan; Ratkai, Zoltan; Seres, Peter; Karancsi, Tamas
 PATENT ASSIGNEE(S): Egis Gyogyszergyar Rt., Hung.
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

AppS

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964402	A1	19991216	WO 1998-HU54	19980605
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9877834	A1	19991230	AU 1998-77834	19980605
EP 1082309	A1	20010314	EP 1998-925869	19980605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2000006183	A	20010130	NO 2000-6183	20001205
PRIORITY APPLN. INFO.:			WO 1998-HU54	A 19980605
OTHER SOURCE(S):		CASREACT 132:22970; MARPAT 132:22970		
AB	Amination of 3,4,5-trichloropyridazine (prepn. given) by H2N(CH2)3OH gave a separable mixt. of 5- and 4-aminated derivs. and the latter was converted to the title compd. in 3 addnl. steps.			
IT 252031-70-2P	RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of 5-chloro-4-[3-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propylamino]-3(2H)-pyridazinone)			
RN 252031-70-2	HCAPLUS			
CN 3(2H)-Pyridazinone, 4-[(3-bromopropyl)amino]-5-chloro-	(9CI) (CA INDEX NAME)			

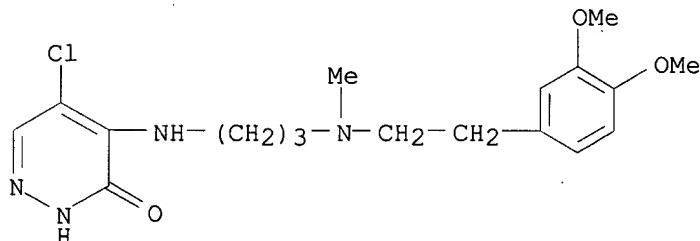


IT 150800-12-7P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**
(Preparation)
(prepn. of 5-chloro-4-[3-[N-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]p
ropylamino]-3(2H)-pyridazinone)

RN 150800-12-7 HCAPLUS

CN 3(2H)-Pyridazinone, 5-chloro-4-[3-[2-(3,4-dimethoxyphenyl)ethyl]methylam
ino]propylamino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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• (FILE 'HOME' ENTERED AT 17:06:00 ON 07 MAR 2002)

FILE 'CASREACT' ENTERED AT 17:06:11 ON 07 MAR 2002

L1 STR
 L2 0 S L1
 L3 1 S L1 FUL, 1 citation (applicant)
 SAVE L3 BER732CR/A

FILE 'REGISTRY' ENTERED AT 17:14:04 ON 07 MAR 2002

L4 STR L1
 L5 1 S L4
 L6 36 S L4 FUL 36 cpds for a str that includes both the
 reactant & product
 SAVE L6 BER732P/A

L7 1 S L6 AND N=3 ← 1 cpd for RCT
 L8 35 S L6 NOT L7 ← 35 cpds for product

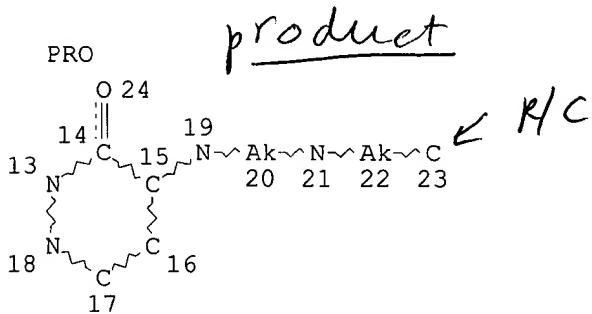
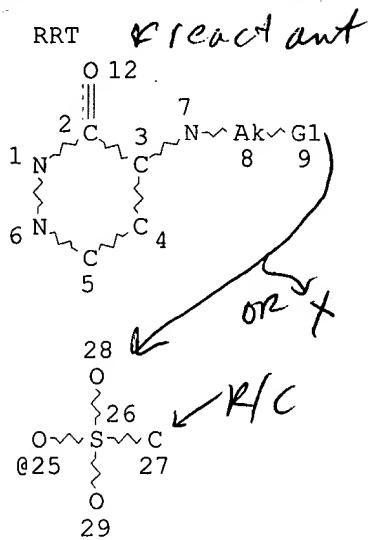
FILE 'HCAPLUS' ENTERED AT 17:29:52 ON 07 MAR 2002

L9 1 S L7/RCT ← 1 cite for RCT
 L10 4 S L8/PREP ← 4 cites for prep
 L11 1 S L9 AND L10 ← 1 cite for RCT & PREP (same as L3)

ca plus search

BERNHARDT 09/701, 732

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L1 STR }

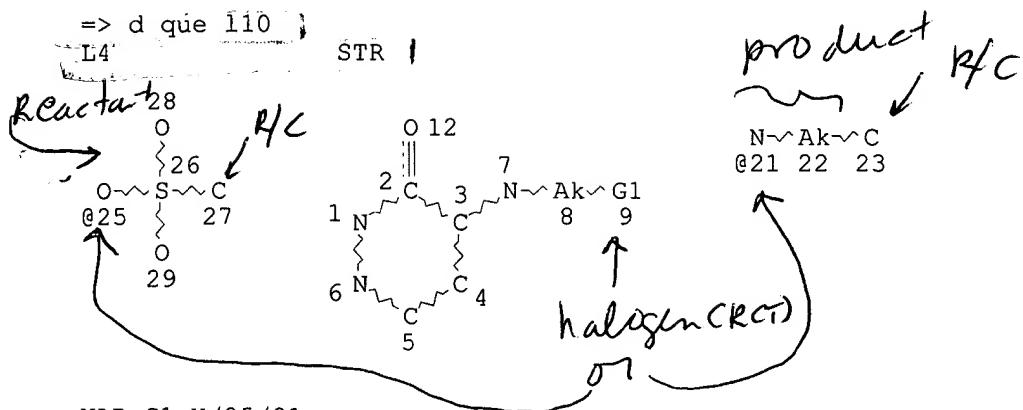


VAR G1=X/25
 NODE ATTRIBUTES:
 NSPEC IS RC AT 23
 NSPEC IS RC AT 27
 CONNECT IS E2 RC AT 1
 CONNECT IS E2 RC AT 6
 CONNECT IS E2 RC AT 13
 CONNECT IS E2 RC AT 18
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS X5 C AT 8
 ECOUNT IS X5 C AT 20
 ECOUNT IS X5 C AT 22

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

*****MAPPINGS*****
 NOD SYM ROL NOD SYM ROL
 7 N RRT 19 N PRO
 19 N PRO 7 N RRT
 L3 1 SEA FILE=CASREACT SSS FUL L1 (1 REACTIONS)



VAR G1=X/25/21

NODE ATTRIBUTES:

NSPEC IS RC AT 23
 NSPEC IS RC AT 27
 CONNECT IS E2 RC AT 1
 CONNECT IS E2 RC AT 6
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS X5 C AT 8
 ECOUNT IS X5 C AT 22

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

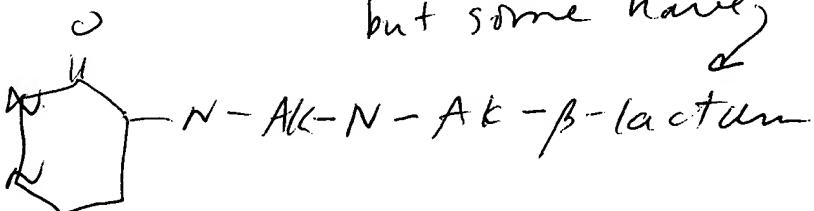
STEREO ATTRIBUTES: NONE

L6 36 SEA FILE=REGISTRY SSS FUL L4
 L7 1 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND N=3
 L8 35 SEA FILE=REGISTRY ABB=ON PLU=ON L6 NOT L7
 L10 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L8/PREP

only 1 cpd fits the reactant
 STR

35 cpds

fit the product
 but some have



correct

BERNHARDT 09/701,732

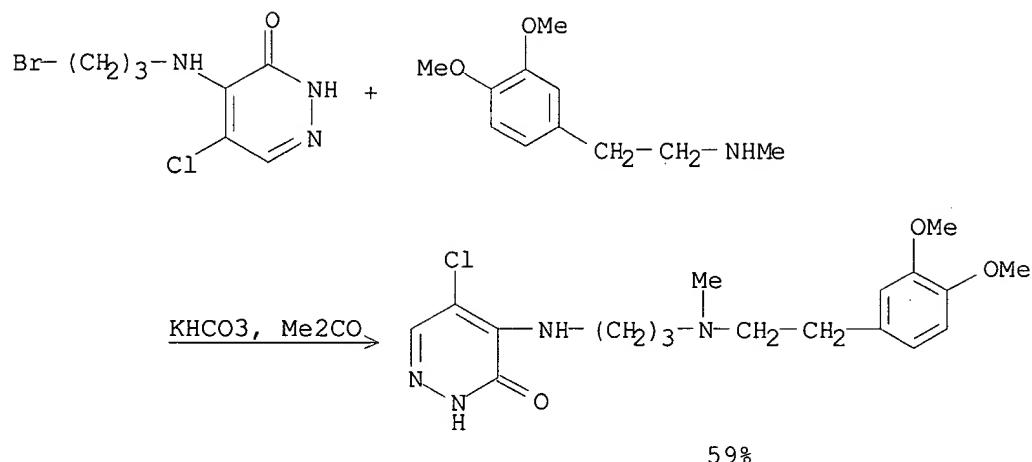
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L3 ANSWER 1 OF 1 CASREACT[®] COPYRIGHT 2002 ACS
ACCESSION NUMBER: 132:22970 CASREACT
TITLE: Preparation of 5-chloro-4-[3-[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propylamino]-3(2H)-pyridazinone
INVENTOR(S): Kotay Nagy, Peter; Simig, Gyula; Barkoczy, Jozsef; Sztruhar, Ilona; Balazz, Laszlo; Doman, Imre; Greff, Zoltan; Ratkai, Zoltan; Seres, Peter; Karancsi, Tamas
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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EP 1082309	A1	20010314	EP 1998-925869	19980605
PRIORITY APPLN. INFO.:			WO 1998-HU54	19980605
OTHER SOURCE(S): MARPAT 132:22970				
AB Amination of 3,4,5-trichloropyridazine (prepn. given) by H2N(CH2)3OH gave a separable mixt. of 5- and 4-aminated derivs. and the latter was converted to the title compd. in 3 addnl. steps.				
NO 2000006183	A	20010130	NO 2000-6183	20001205

App's

RX(3) OF 15



REF: PCT Int. Appl., 9964402, 16 Dec 1999

REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT